Dynamics of superfluid ^{4}He: Single– and multiparticle excitations

Dec. 7, 2016

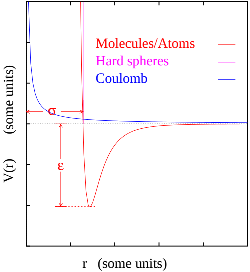
Theory: C. E. Campbell, E. Krotscheck, T. Lichtenegger
Experiments: Ketty Beauvois, Björn Fåk, Henri Godfrin, Hans Lauter, Jacues Olivier, Ahmad Sultan...

Sub-eV, Dec. 7-9, 2016

Outline

How "quantum" is a (quantum) liquid ?

Let $V_{JL}(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$



$$x = \frac{r}{\sigma} \quad V_{LJ}(r) = \epsilon\, v(x)$$

Then $\frac{1}{\epsilon}H(\mathbf{x}_1 \ldots, \mathbf{x}_N) = -\frac{\Lambda^2}{2}\sum_i \nabla^2_{\mathbf{x}_i} + \sum_{i<j} v(|\mathbf{x}_i - \mathbf{x}_j|)$

Quantum Parameter: $\Lambda = \left(\frac{\hbar^2}{m\epsilon\sigma^2}\right)^{\frac{1}{2}}$

$\Lambda \approx 3$ for He, $\Lambda \approx 1-2$ for H_2, HD, D_2, $\Lambda < 0.1$ for rare gases.

- Double differential cross section: What experimentalists measure

$$\frac{\partial^2\sigma}{\partial\mathbf{\Omega}\,\partial\hbar\omega} = b^2\left(\frac{k_f}{k_i}\right)S(\mathbf{k},\hbar\omega)$$

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- Dynamic structure function: The definitions

$$S(\mathbf{k}, \hbar\omega) = \frac{1}{N} \sum_n \left| \left\langle \Psi_n \middle| \rho_{\mathbf{k}} \middle| \Psi_0 \right\rangle \right|^2 \delta(\hbar\omega - \varepsilon_n)$$

$$H \big| \Psi_0 \big\rangle = E_0 \big| \Psi_0 \big\rangle \qquad H \big| \Psi_n \big\rangle = [E_0 + \varepsilon_n] \, \big| \Psi_n \big\rangle$$

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- Density-density response function: What theorists calculate

$$\begin{aligned} S(\mathbf{k},\hbar\omega) &= -\frac{1}{\pi}\Im m\,\chi(\mathbf{k},\hbar\omega) \\ \delta\rho_1(\mathbf{r},t) &= \int d^3r'dt'\;\chi(\mathbf{r},\mathbf{r}';t-t')\delta V_{ext}(\mathbf{r}',t') \end{aligned}$$

Early experiments

R. A. Cowley and A. D. B. Woods, Can. J. Phys. **49**, 177 (1971).

Spectrum by Cowley and Woods 1971

COWLEY AND WOODS: INELASTIC SCATTERING OF THERMAL NEUTRONS FROM LIQUID HELIUM

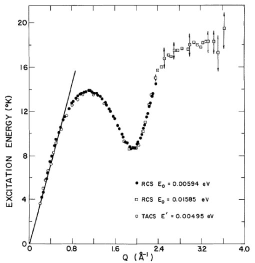

FIG. 7. The experimental results for the energies of the one-phonon excitations at 1.1 °K.

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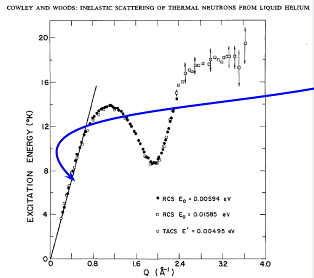

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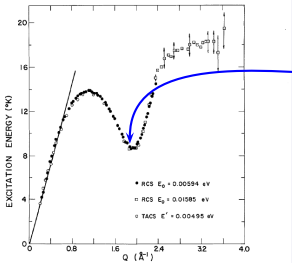

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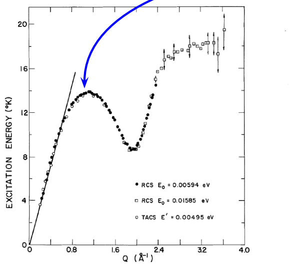

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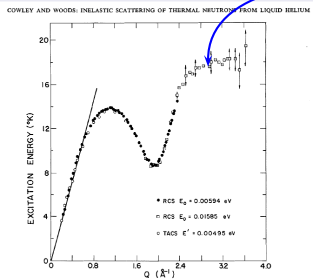

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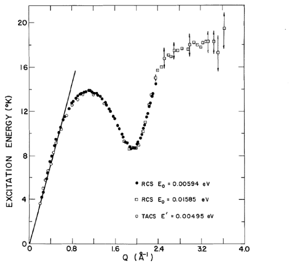

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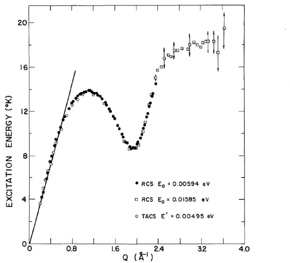

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- Is there anything else to be seen ?

The theorist's tools:

$$H(t)\left|\psi(t)\right\rangle = i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle$$

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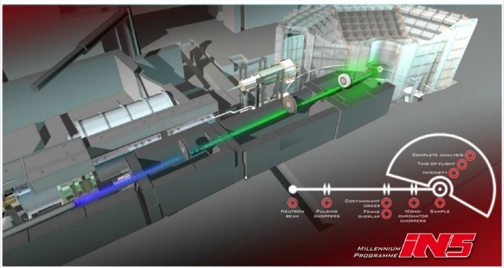

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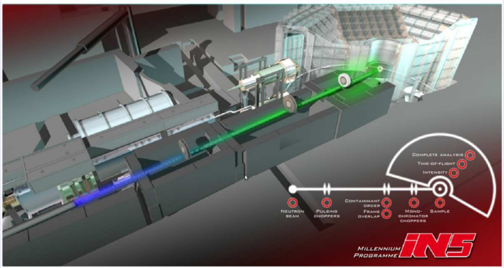

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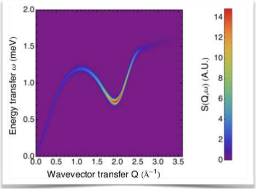

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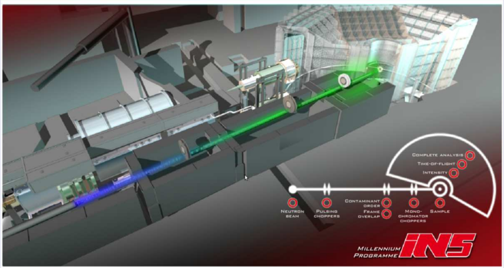

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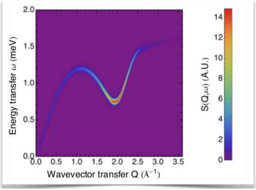

Is there anything else to be seen ?

Postulate...

1. An empirical, non-relativistic microscopic Hamiltonian

$$H = -\sum_i \frac{\hbar^2}{2m}\nabla_i^2 + \sum_i V_{\text{ext}}(i) + \sum_{i<j} V(i,j)$$

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6. Phase transitions (?)...

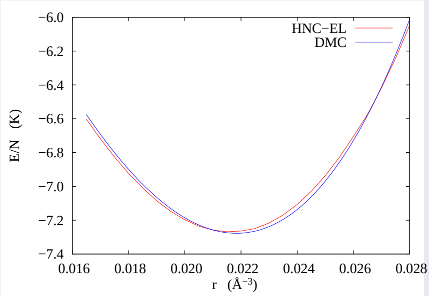
A “simple quick and dirty” method:

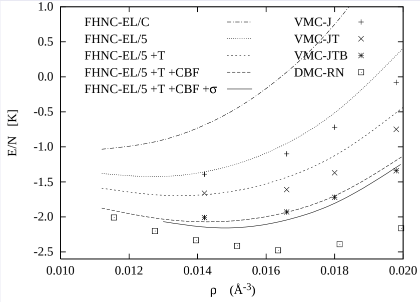
$$\Psi_0(1,\ldots,N) = \exp\frac{1}{2}\left[\sum_i u_1(\mathbf{r}_i) + \sum_{i<j} u_2(\mathbf{r}_i,\mathbf{r}_j) + \ldots\right]\Phi_0(1,\ldots,N)$$

$$\equiv F(1,\ldots,N)\Phi_0(1,\ldots,N)$$

$\Phi_0(1,\ldots,N)$ “Model wave function” (Slater determinant)

Equation of state for ^{4}He and ^{3}He:





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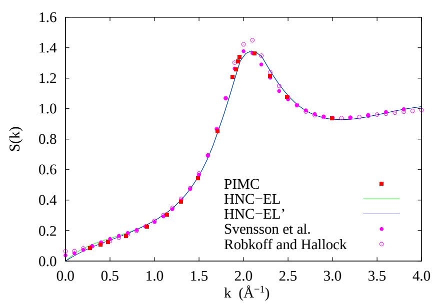
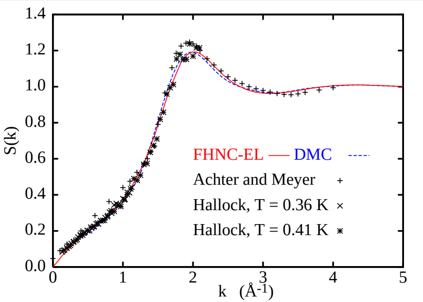
Structure functions of ^{4}He and ^{3}He





Build on the success story for the ground state:
Make the correlations time dependent !

$$|\Phi(t)\rangle = e^{-iE_0 t/\hbar} \frac{1}{\mathcal{N}(t)} F e^{\frac{1}{2}\delta U} |\Phi_0\rangle \ ,$$

$|\Phi_0\rangle$: model ground state, $\delta U(t)$: excitation operator, $\mathcal{N}(t)$: normalization.
Bosons:

$$\delta U(t) = \sum_i \delta u^{(1)}(\mathbf{r}_i;t) + \sum_{i<j} \delta u^{(2)}(\mathbf{r}_i,\mathbf{r}_j;t) + \ldots$$

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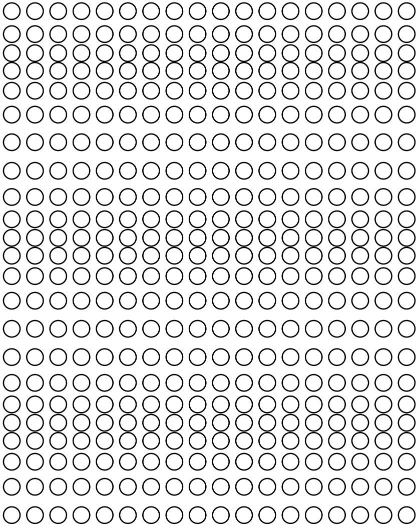
- $\delta u^{(2)}$ describes fluctuations of the short-ranged structure
- The physical content of $\delta u^{(2)}$ is beyond mean field theory !

$$\delta U(t) = \sum_i \delta u^{(1)}(\mathbf{r}_i;t)$$



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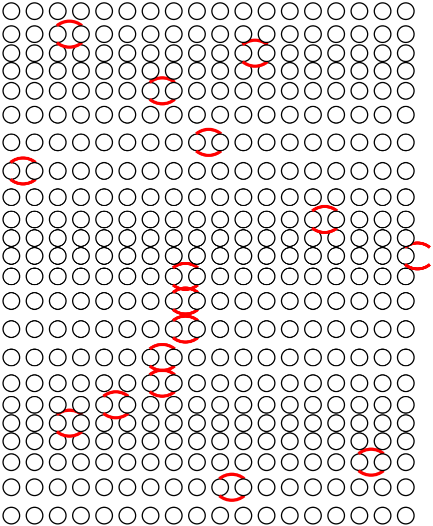

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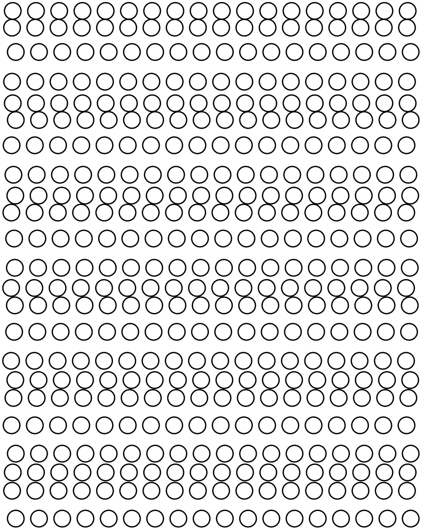

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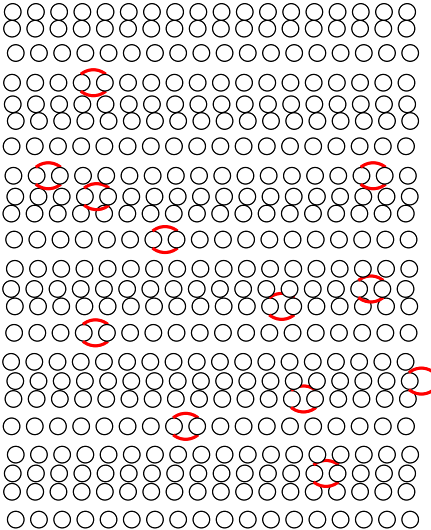
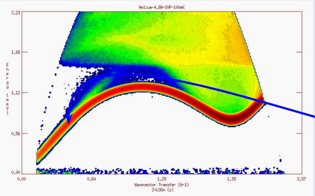
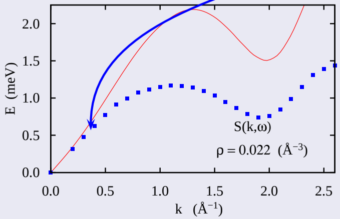


Experiments



Feynman (RPA)-Theory



One-body fluctuations:
Feynman(RPA) spectrum

$$\delta U(t) = \sum_i e^{i(\mathbf{k}\cdot\mathbf{r}_i - \omega t)}$$

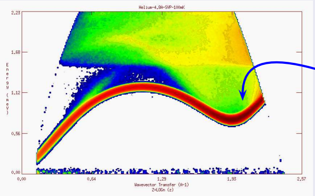
$$\hbar\omega(k) = \hbar^2 k^2 / 2mS(k)$$

$$\hbar\omega(k) = ck \quad \text{as} \quad k \to 0$$

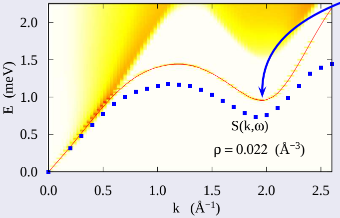
Bosons: ^{4}He in 3D

Confronting Theory and Experiment: Experiments by Godfrin group in Grenoble

Experiments



Single-Pair-Fluctuations



Two-body fluctuations:

Feynman-Cohen "backflow"

$$\delta U(t) = \sum_i e^{i(\mathbf{k}\cdot\tilde{\mathbf{r}}_i - \omega t)}$$

$$\tilde{\mathbf{r}}_i = \mathbf{r}_i + \sum_{j\neq i} \eta(r_{ij})\mathbf{r}_{ij}$$

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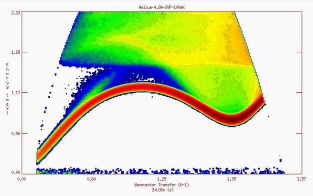
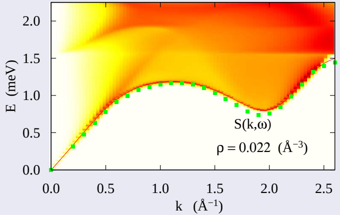


Multi-Pair-Fluctuations



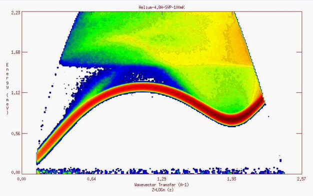
Many-body fluctuations:

- $$\begin{aligned}\delta U(t) &= \sum_i \delta u^{(1)}(\mathbf{r}_i;t)\\ &+ \sum_{i<j} \delta u^{(2)}(\mathbf{r}_i,\mathbf{r}_j;t) + \ldots\end{aligned}$$

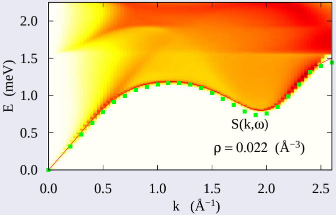
  Stationarity principle

$$\delta \int dt \left\langle \Phi(t) \middle| H + \delta H(t) - i\hbar\frac{\partial}{\partial t} \middle| \Phi(t) \right\rangle = 0$$

Experiments



Multi-Pair-Fluctuations



Many-body fluctuations:

- $$\delta U(t) = \sum_i \delta u^{(1)}(\mathbf{r}_i; t) + \sum_{i<j} \delta u^{(2)}(\mathbf{r}_i, \mathbf{r}_j; t) + \ldots$$

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  $$\delta \int dt \left\langle \Phi(t) \middle| H + \delta H(t) - i\hbar \frac{\partial}{\partial t} \middle| \Phi(t) \right\rangle = 0$$

- Brillouin-Wigner perturbation theory in the basis $\{e^{i\sum_i \mathbf{k}\cdot\mathbf{r}_i} | \Psi_0 \rangle\}$.

- Dynamic Structure Function

$$S(\mathbf{k},\omega) = -\frac{1}{\pi}\Im m \int d^3 r e^{i\mathbf{k}\cdot\mathbf{r})}\chi(\mathbf{r},\mathbf{r}';\omega).$$

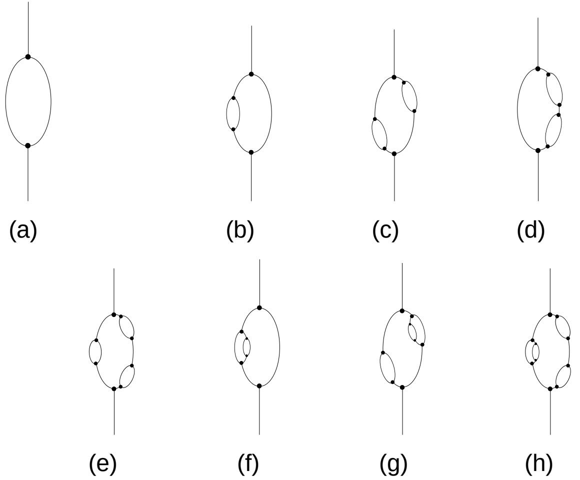
- Density–density response function

$$\chi(k,\omega) = \frac{S(k)}{\omega - \Sigma(k,\omega)} + \frac{S(k)}{-\omega - \Sigma(k,-\omega)} ,$$

- Self-energy

$$\Sigma(k,\omega) = \varepsilon_0(k) + \frac{1}{2}\int \frac{d^3p d^3q}{(2\pi)^3\rho} \frac{\delta(\mathbf{k}-\mathbf{p}-\mathbf{q})\left|V_3(\mathbf{k};\mathbf{p},\mathbf{q})\right|^2}{\omega - \Sigma(p,\omega-\varepsilon_0(q)) - \Sigma(q,\omega-\varepsilon_0(p))}$$

- 3-phonon vertex $V_3(\mathbf{k};\mathbf{p},\mathbf{q})$


(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)

- Is it

Quantum Statistical Mechanics in the Natural Sciences
Studies in the Natural Sciences Volume 4, 1974, pp 359-402

The Ghost of a Vanished Vortex Ring

Russell J. Donnelly

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- Or

Is the Roton in Superfluid ^{4}He the Ghost of a Bragg Spot?*

P. Nozières

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Centre National de la Recherche Scientifique,
B.P.166, 38042 Grenoble Cedex 9, France
E-mail: nozieres@ill.fr

The physical mechanisms
What is a roton ?

- Is it

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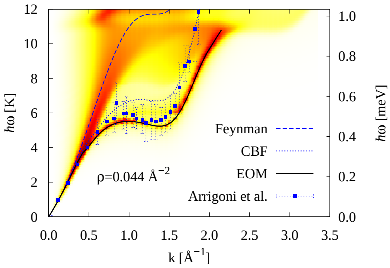
- If so, could there be a second Bragg peak ?
(None found in 3D ^{4}He)

- Below saturation ($\rho = 0.044\,\text{Å}^{-2}$) strong anomalous dispersion;



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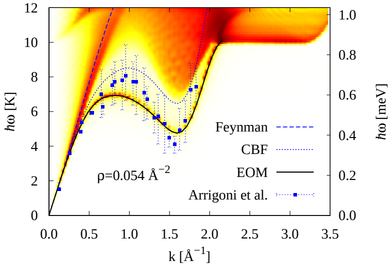
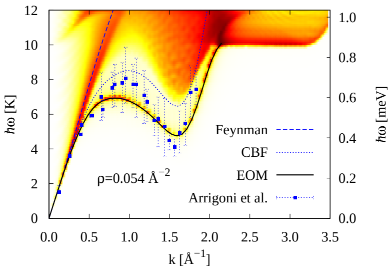


- Below saturation ($\rho = 0.044\,\text{Å}^{-2}$) strong anomalous dispersion;
- Roton paramaters within error bars of Monte Carlo calculations;
- Around saturation, not much new;



- Below saturation ($\rho = 0.044\,\text{Å}^{-2}$) strong anomalous dispersion;
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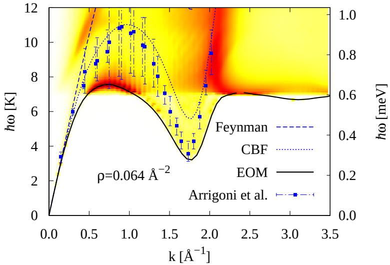
- Close to the liquid-solid phase transition, a weak, secondary "roton" !



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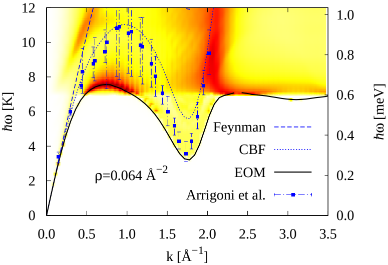

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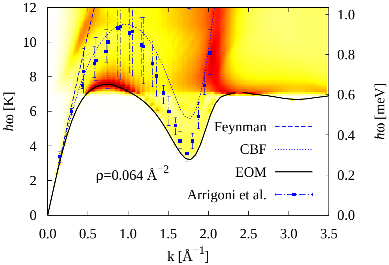
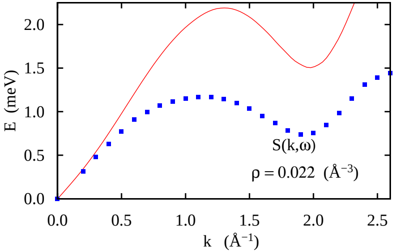
- Roton paramaters within error bars of Monte Carlo calculations;
- Around saturation, not much new;
- Close to the liquid-solid phase transition, a weak, secondary "roton" !
- Monte Carlo calculations dynamically inconsistent
- Still a challenge for neutron scatterer !



- Sum rules

$$\int d\omega \Im m \chi(k,\omega) = S(k)$$

$$\int d\omega \omega \Im m \chi(k,\omega) = \frac{\hbar^2 k^2}{2m}$$



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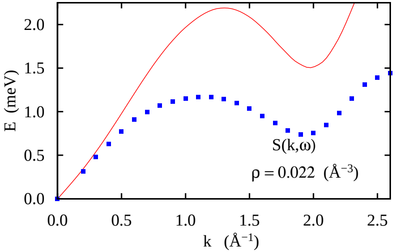
- If we assume only one phonon, we get Feynman (off by a factor of 2)



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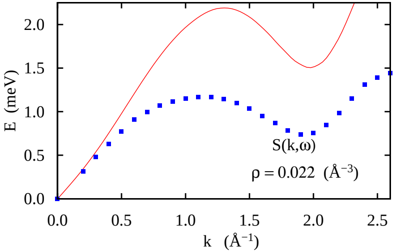
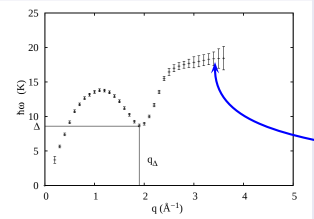
- If we assume only one phonon, we get Feynman (off by a factor of 2)
- Need a multi(quasi-)particle continuum to get the energetics right !

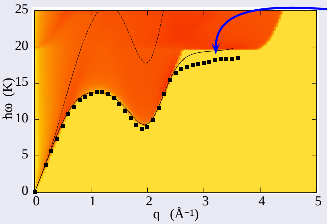


The physical mechanisms:
Mode-mode couplings

Experiments



Theory



The "Pitaevskii plateau"

A perturbation with momentum **q** and energy ω can decay into two rotons $\mathbf{q}_\Delta^{(1)}$ and $\mathbf{q}_\Delta^{(2)}$ with $|\mathbf{q}_\Delta^{(1)}| = |\mathbf{q}_\Delta^{(2)}| = q_\Delta$ under momentum and energy and conservation $\omega = 2\Delta$.

- The roton momenta may be aligned

$$|\mathbf{q}| \leq 2q_R$$

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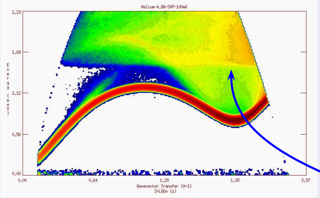

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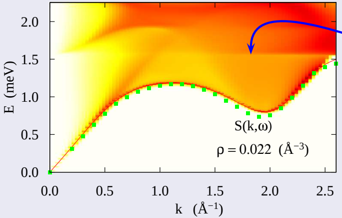

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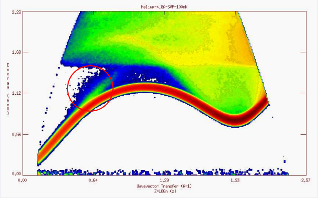
- The roton momenta may be aligned

$$|\mathbf{q}| \leq 2q_R$$

- or anti-aligned

$$|\mathbf{q}| \geq 0$$

Experiments



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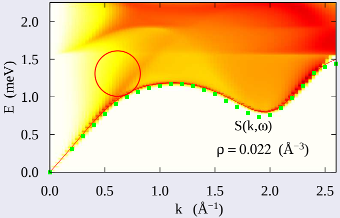

The "ghost phonon"

Phonon dispersion relation

$$\omega(q) = cq(1+\gamma q^2)$$

- "normal dispersion": $\gamma < 0$
  $\Rightarrow$ phonons are stable
- "anomalous dispersion": $\gamma > 0$
  $\Rightarrow$ phonons can decay

$\Rightarrow$ ^{4}He at zero pressure is borderline between normal and anomalous, $\gamma \approx 0.1$

$\Rightarrow$ Perturbations with momentum ($\mathbf{q}$, ω) can decay into two phonons with ($\mathbf{q}/2$, $\omega/2$) as long as the dispersion relation is almost linear up to $q/2$.

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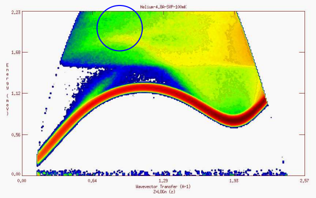

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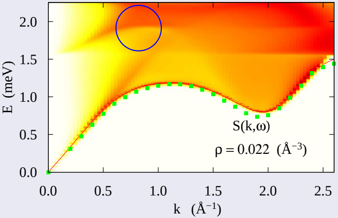

Maxon-roton coupling

A similar but less sharply defined process

What we know today

- Quantitative agreement between experiments in 3D;

Summary

What we know today

- Quantitative agreement between experiments in 3D;
- Prediction of a secondary roton–like mode in 2D ^{4}He;

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Summary

What we know today

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- Prediction of maxon damping at high pressure ^{4}He
- Structures are more pronounced in 2D;

Summary

What we know today

- Quantitative agreement between experiments in 3D;
- Prediction of a secondary roton–like mode in 2D ^{4}He;
- Prediction of maxon damping at high pressure ^{4}He
- Structures are more pronounced in 2D;
- $1 \to 2$ and $2 \to 1$ processes are not the end of the story but do not lead to sharp features.

Thanks to collaborators in this project

C. E. Campbell	Univ. Minnesota
F. M. Gasparini	University at Buffalo
H. Godfrin (and his team)	CNRS Grenoble
T. Lichtenegger	University at Buffalo

Thanks for your attention

and thanks to our funding agency:

FWF

Der Wissenschaftsfonds.